Reversible stretching of a short peptide using parallel adaptive biasing force simulations

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The adaptive biasing force (ABF) scheme is a powerful molecular dynamics based method for overcoming the barriers of the free energy landscape. Integration of the average force measured along a chosen model reaction coordinate (RC) yield the so-called potential of mean force. The mean force that acts at any given point of the discretized model RC is estimated by accruing and averaging the instantaneous force exerted on the system. Faster exploration of the reaction pathway can be achieved by running multiple replicas in parallel and exchanging information at fixed intervals in the course of the simulation. Numerical simulations performed on the prototypical deca-alanine peptide globally improve the convergence properties of the free-energy calculation through a more efficient exploration of compact configurations reflected in parallel valleys of the free-energy landscape. Diffusion along the model RC is further enhanced by a selection mechanism, whereby far-reaching replicas are cloned, replacing less effective walkers.